3-D Structure at Atomic Resolution by High-Tilt Electron Microscopy

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By processing multiple series of high-resolution electron microscope images, scientists at UC Berkeley and LBNL have produced three-dimensional potential maps of mineral specimens. These maps reveal the positions of all the atoms in the structure, including light atoms such as oxygen that are not detectable in ordinary two-dimensional micrographs.

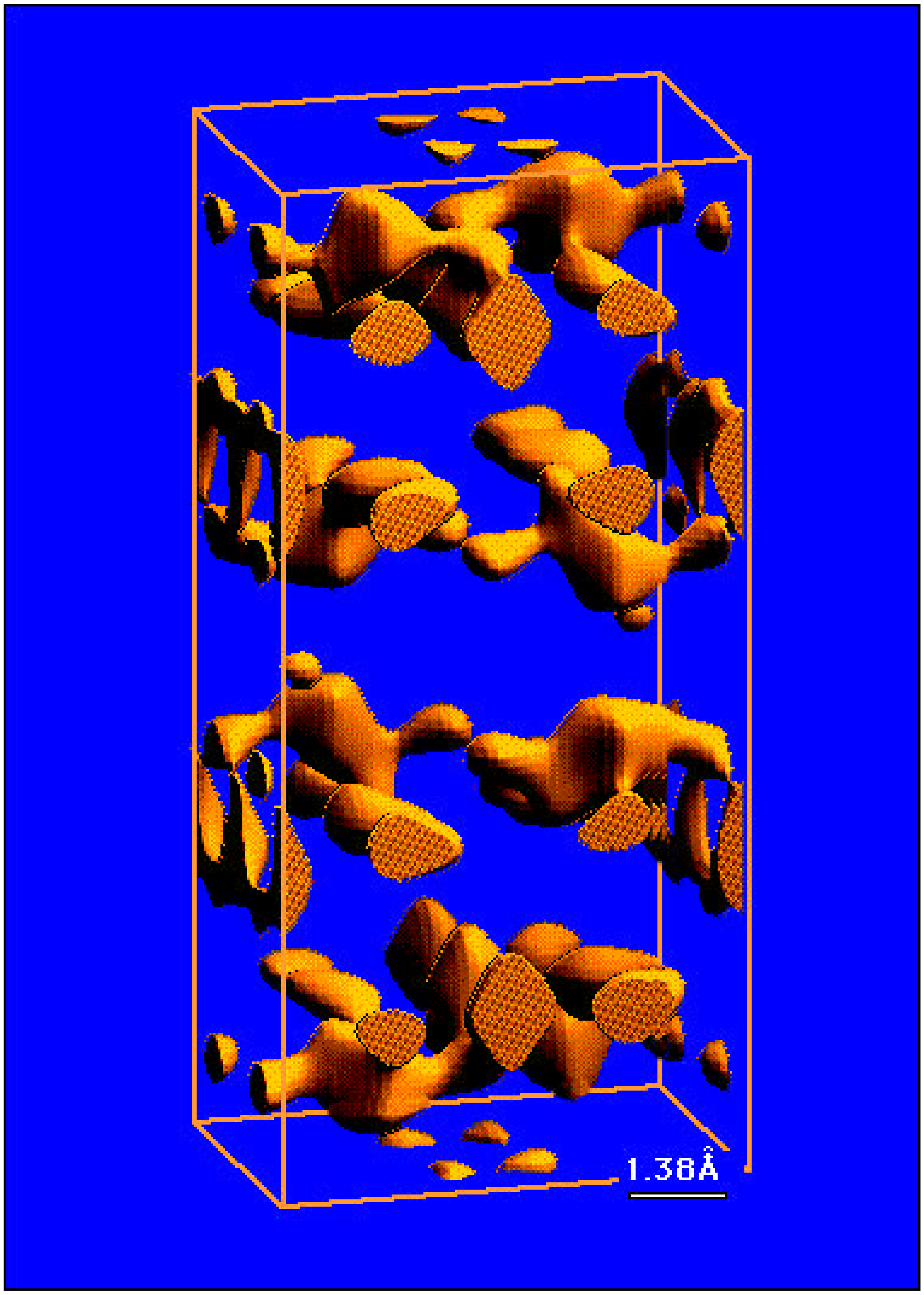
Background - Biologists use reconstruction from electron microscope images to produce three-dimensional models at resolutions that reveal "clumps" of unresolved atoms. Materials scientists work from images with resolution that is sufficiently good to show spacings smaller than some atomic bond distances (thus resolving pairs of atoms, or even individual atoms). But these images are two-dimensional projections through the specimen structure, and the superposition of atoms in different layers produces images with a confusing overlap of atomic detail. By using three-dimensional reconstruction at atomic resolution, it was hoped to produce a three-dimensional map of the specimen potential that would reveal individual atoms.

Accomplishment - An unusual collaboration of researchers from different disciplines combined techniques used in biology with those used in materials science. Using a method of three-dimensional reconstruction that was developed by biologists and has been used for images of proteins at resolutions down to 3.5Å, the team of scientists processed high-resolution images of the mineral staurolite. The images were obtained at resolutions down to 1.38Å on the Berkeley atomic-resolution microscope (ARM). Three-dimensional reconstruction requires the ability to obtain series of electron microscope images along several different directions, and thus requires the ability to tilt the specimen over large angles within the microscope. The ARM permits specimen tilts of ±40° around two perpendicular axes.

The researchers obtained focal-series of images along three mutually perpendicular directions, and, by taking advantage of the unique high-angle tilt capability of the Berkeley atomic-resolution electron microscope, in two other major crystallographic directions. Initial results were at a resolution of 1.6Å, using just one image in each of the five crystallographic directions that were accessible by tilting [1]. Later [2] an implementation of a method that used processing of focal series of images to increase the resolution allowed the use of a series of up to ten images (each at a different focus value) from each crystallographic direction, improving the resolution in the three-dimensional reconstruction from 1.6Å to 1.38Å.

The result of the image processing and three-dimensional reconstruction is a three-dimensional map of the Coulomb potential within the unit cell of the specimen structure. A surface of constant potential, derived from the map and displaying a level selected to show the "surfaces" of the atoms, is shown in the figure.

"Images" formed by taking slices through the three-dimensional Coulomb potential reveal all the atoms that lie in the plane of the slice, since the resolution in the potential map is better than the bond-length. Such "images" avoid the confused super-position present in a conventional micrograph, since any slice is a *section* through the structure, whereas a conventional electron micrograph is a *projection* of the structure.



Three-dimensional view of the atomic structure of staurolite. The figure shows a Coulomb potential surface that is adjusted to be at a level that reveals the positions of the silicon, aluminum and oxygen atoms that make up the unit cell (outlined). The view is oblique along the z axis.

1. K.H. Downing, H. Meisheng, H.R. Wenk and M. A. O'Keefe, *Nature* 348 (1990) 525-528.
2. H.-R. Wenk, K.H. Downing, H. Meisheng, and M.A. O'Keefe, *Acta Cryst*. A48 (1992) 700-716.